

Supporting Information

Incorporating Fast Protein Dynamics into Enzyme Design:

A Proposed Mutant Aromatic Amine Dehydrogenase

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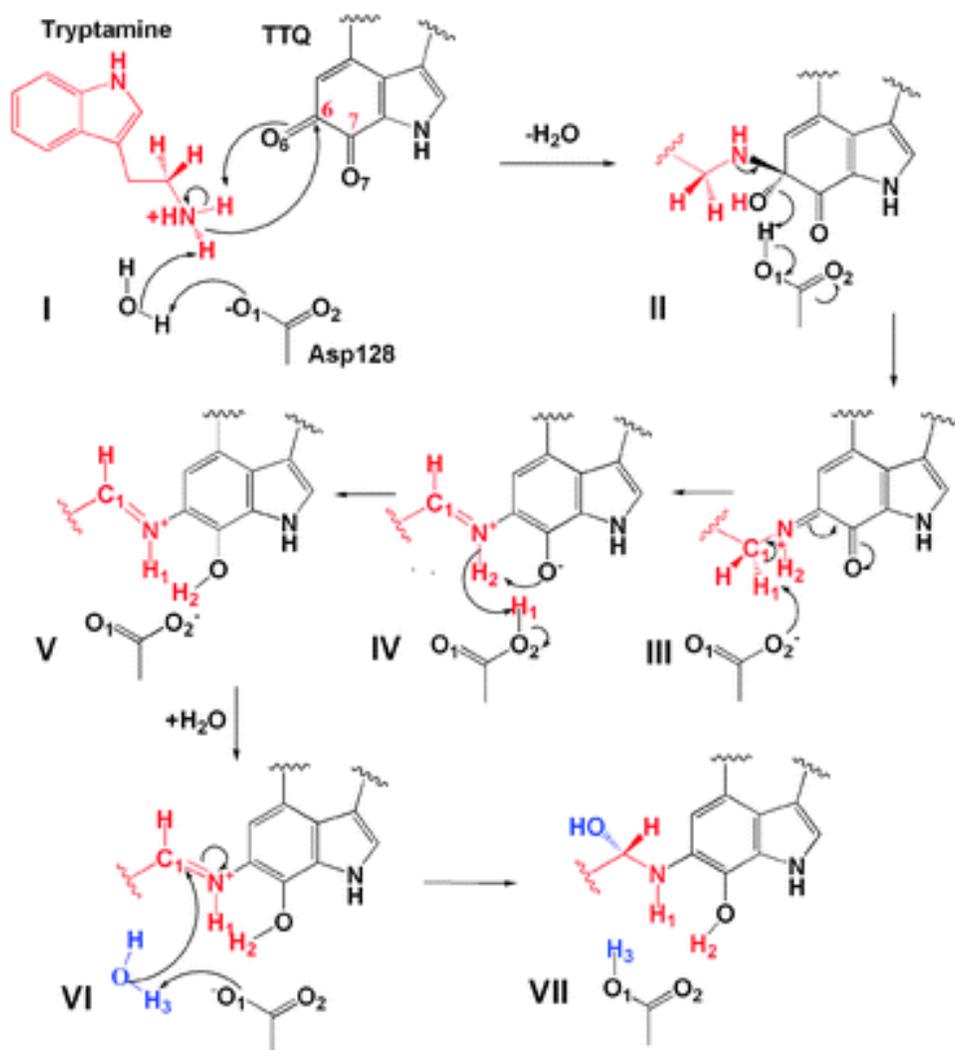
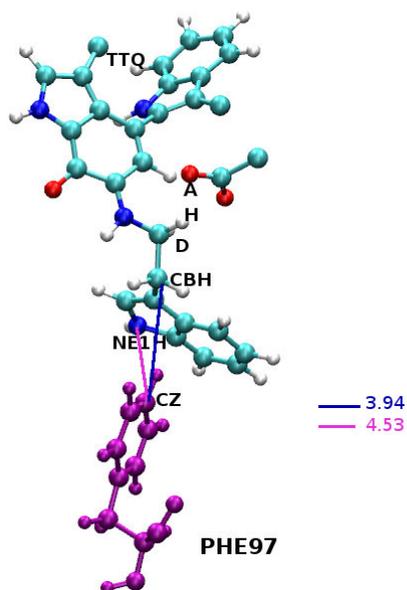


Figure S1: Reaction mechanism of the reductive half-reaction of AADH with tryptamine.

A



B

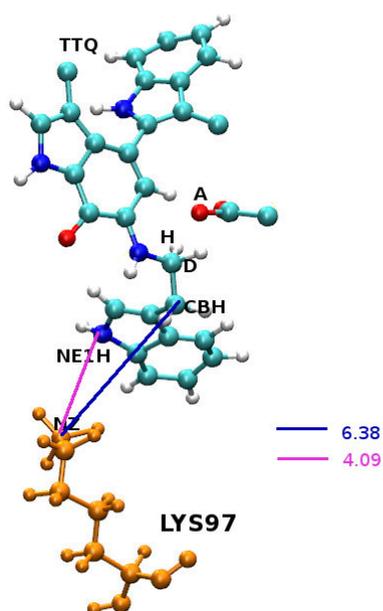


Figure S2: (A) WT AADH starting structure of the active site and residue PHE97, (B) F97K AADH starting structure of the active site and residue mutated to LYS97.

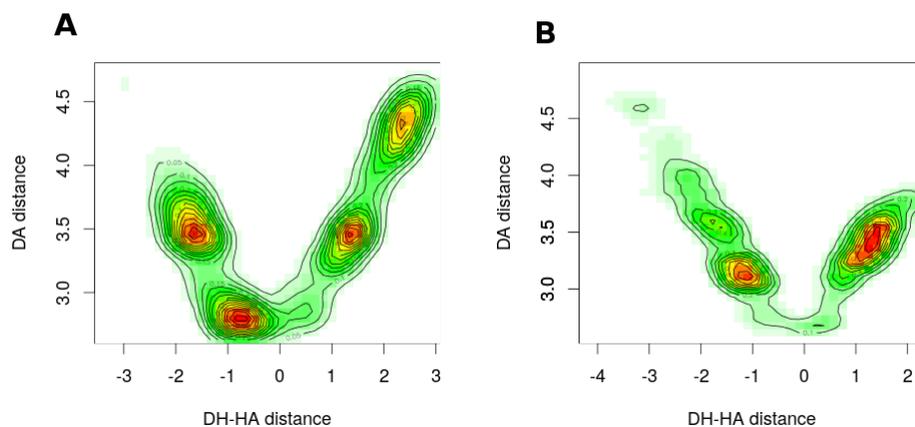


Figure S3: Projections of histogrammed densities of the structures along all reaction trajectories on the plane of the donor–acceptor vs bond breaking (D–H) minus bond forming (H–A) distance, for WT AADH (a) and F97K AADH (b). The colormap (white for “plains”, i.e. zero density, up to red for “mountains”, i.e. maximum density of structures) represents the allocation of a pair of the above geometric properties among structures along the reaction path. Contour maps that join points with equal density have also been drawn. Note that the F97K achieves a shorter minimum D–A distance right at the TS.

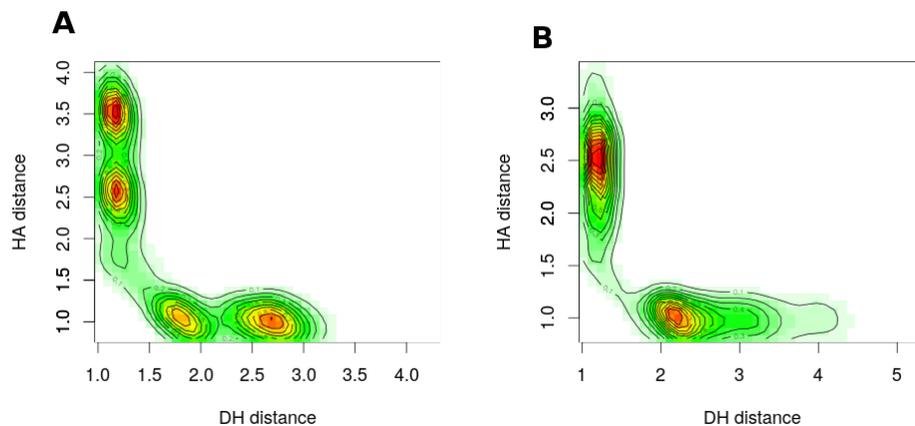


Figure S4: Reactive trajectories projected on the plane of bond-breaking and bond-forming distances, for WT AADH (a) and F97K AADH (b). The colormap (white for “plains”, i.e. zero density, up to red for “mountains”, i.e. maximum density of structures) represents the allocation of a pair of the above geometric properties among structures along the reaction path. Contour maps that join points with equal density have also been drawn. Note that the D–H, H–A distances at the TS for the mutant are shorter than in the WT.

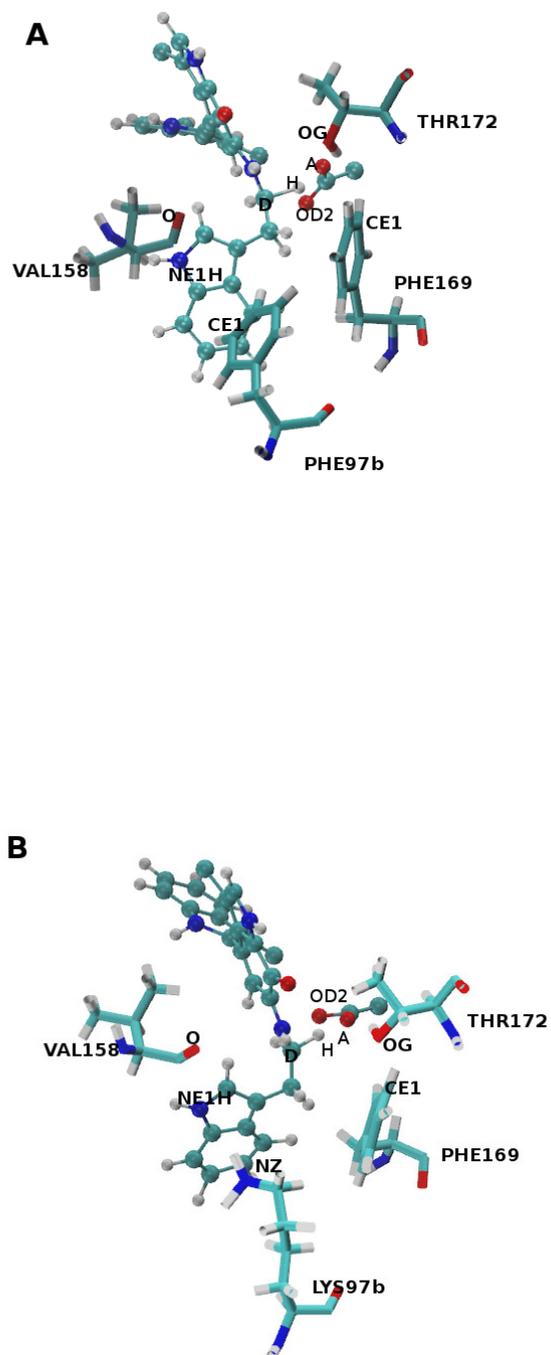


Figure S5: Representative TS structures, including QM region and residues 169,158,97,172 for (A) WT AADH and (B) F97K AADH.

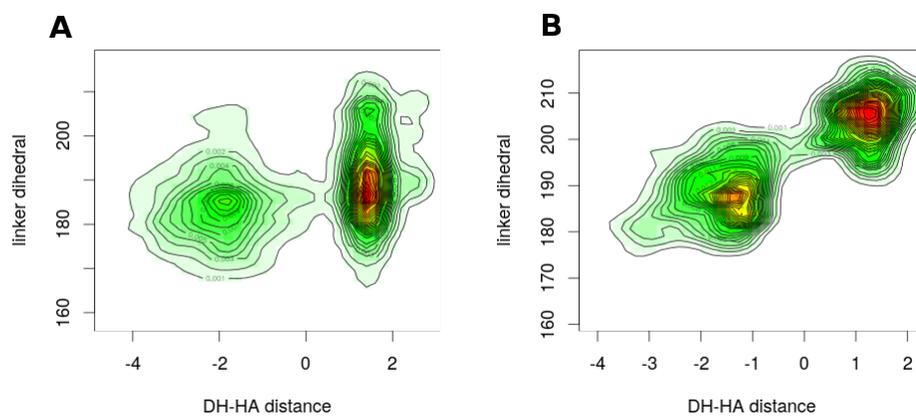


Figure S6: Projections of histogrammed densities of the structures along all reaction trajectories on the plane of the linker angle vs bond breaking (D–H) minus bond forming (H–A) distance, for WT AADH (a) and F97K AADH (b). The colormap (white for “plains”, i.e. zero density, up to red for “mountains”, i.e. maximum density of structures) represents the allocation of a pair of the above geometric properties among structures along the reaction path. Contour maps that join points with equal density have also been drawn.